

# 5-sec-butyl-3-methyl-2-(methylthio)pyrazine

**Inchi:** InChI=1S/C10H16N2S/c1-5-7(2)9-6-11-10(13-4)8(3)12-9/h6-7H,5H2,1-4H3  
**InchiKey:** IUMMRLGFGJURKP-UHFFFAOYSA-N  
**Formula:** C10H16N2S  
**SMILES:** CCC(C)c1cnc(SC)c(C)n1  
**Mol. weight [g/mol]:** 196.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	3.020		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38729&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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